Supplementary Information for

"Shear Induced Deformation Twinning Evolution in Thermoelectric InSb"

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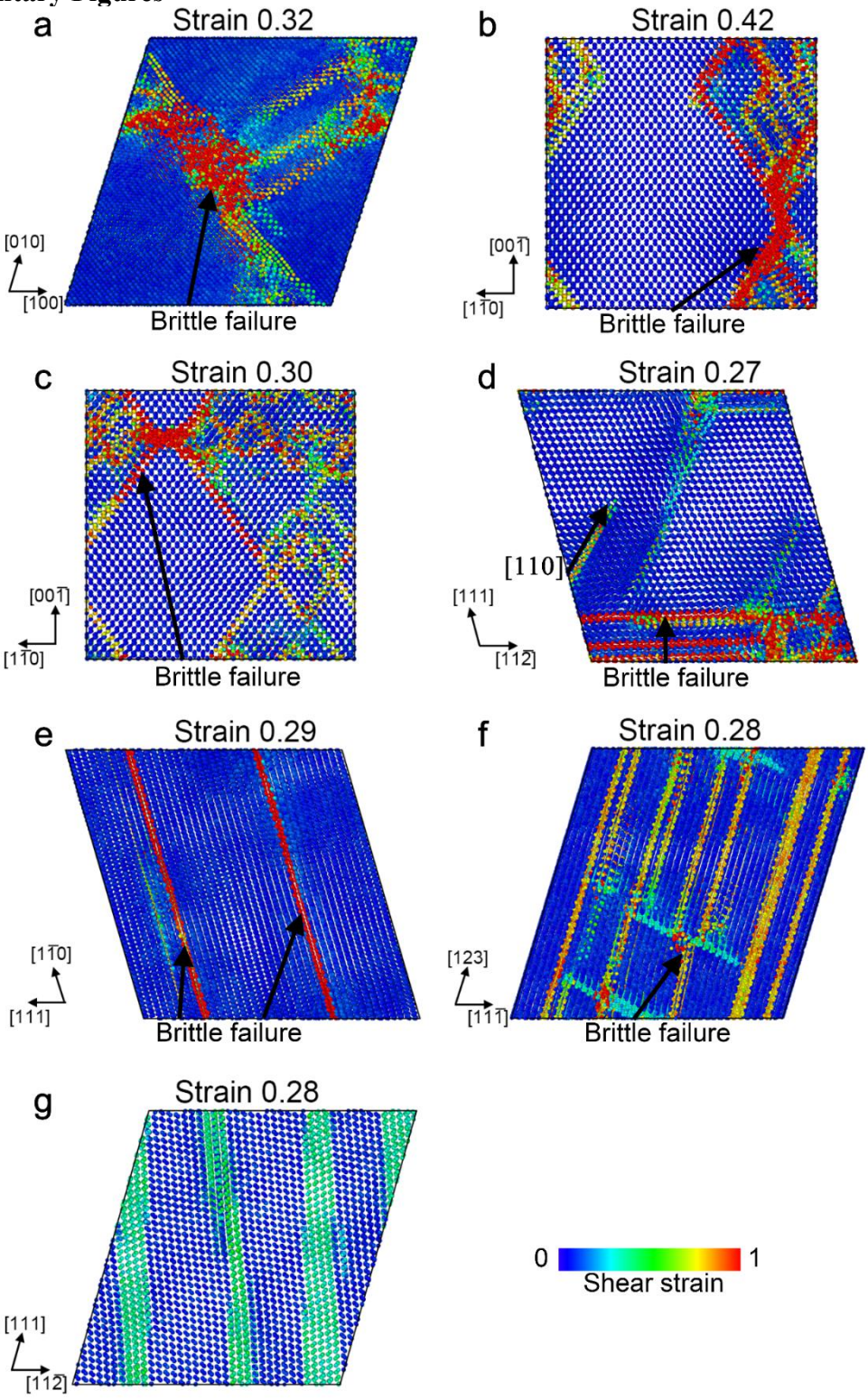
Supplementary Table

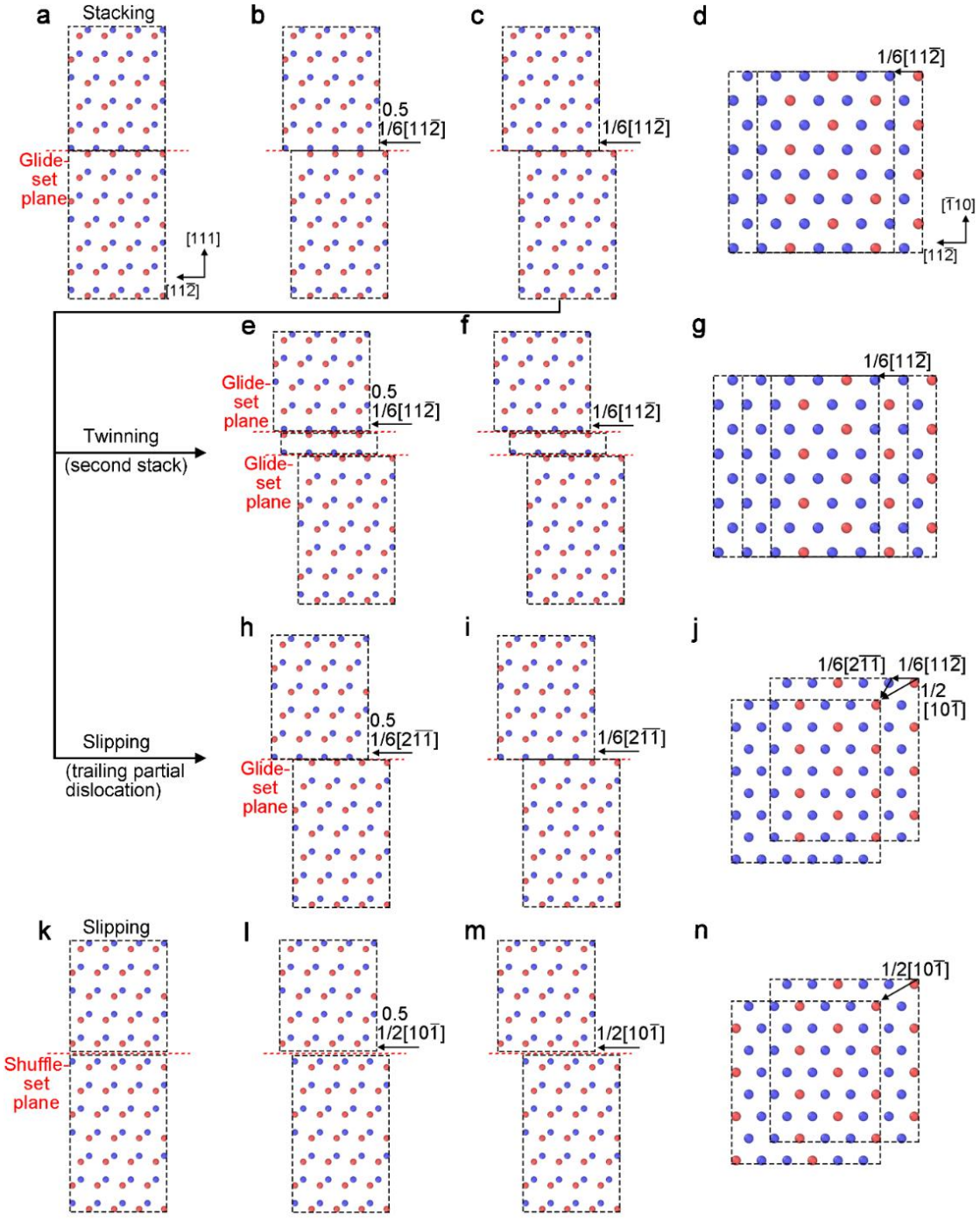
Supplementary Table 1| Direction and size of InSb single crystal models, and shear direction.

Coordinate direction (x×y×z)	Supercell size (x×y×z) (Å)	Atoms number	Shear direction
[100]×[010]×[001]	142.5×142.5×142.5	85184	(010)[100]
[110]×[1$\bar{1}$0]×[00$\bar{1}$]	142.0×142.0×142.5	84568	(00$\bar{1}$)[110] (1$\bar{1}$0)[110]
[11$\bar{2}$]×[111]×[1$\bar{1}$0]	142.8×145.9×142.0	87048	(111)[11$\bar{2}$] (111)[$\bar{1}\bar{1}$2] (1$\bar{1}$0)[111]
[11$\bar{1}$]×[123]×[5$\bar{4}$1]	145.9×145.4×147.0	91728	(123)[11$\bar{1}$]

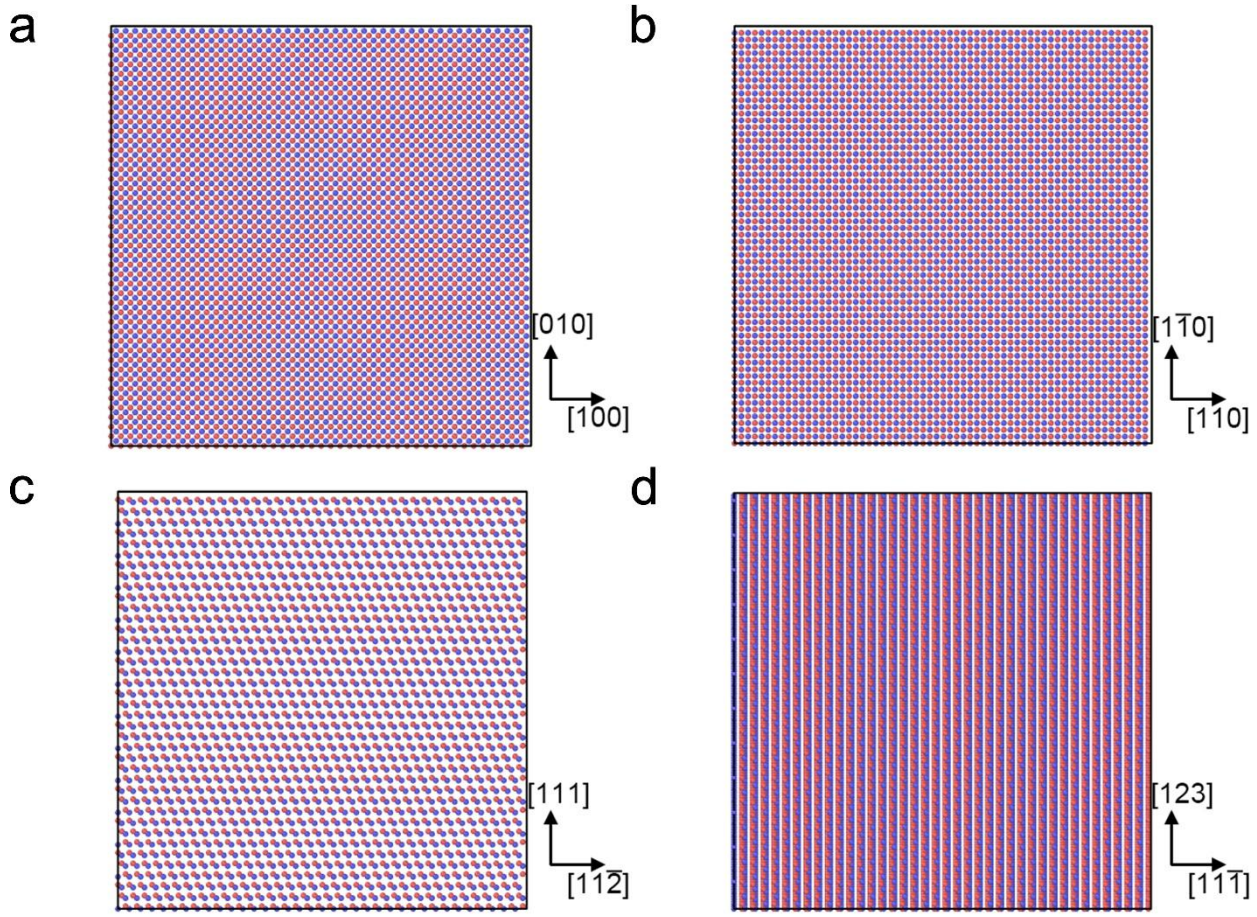
Supplementary Figures



Supplementary Figure 1| Structural deformation along different slip systems. Structural deformation beyond maximum stress point along different slip systems. (a)-(g): Structural deformation beyond maximum stress point along (a) (010)[100] slip system, (b) $(1\bar{1}0)[110]$ slip system, (c) $(00\bar{1})[110]$ slip system, (d) $(111)[\bar{1}\bar{1}2]$ slip system, (e) $(1\bar{1}0)[111]$ slip system, (f) $(123)[11\bar{1}]$ slip system, (g) $(111)[11\bar{2}]$ slip system. Atoms are colored coded by the atomic shear strain. Red atoms indicate that there is breakage, the $(111)[11\bar{2}]$ slip system is the only one that does not fail beyond maximum stress point.



Supplementary Figure 2| Processes of different shear deformation modes on {111} planes. Processes of stacking, twinning, and slipping on glide-set planes and shuffle-set planes. (a)-(c): The process of stacking induced by a leading partial dislocation on glide-set plane. (d) The projection of (c) on (111) plane. (e) and (f): The process of twinning induced by another similar partial dislocation on an adjacent glide-set plane. (g) The projection of (f) on (111) plane. (h) and (i): The process of slipping induced by a trailing partial dislocation on the same glide-set plane. (j) The projection of (i) on (111) plane. (k)-(m): The process of slipping induced by a perfect dislocation on shuffle-set plane. (n) The projection of (m) on (111) plane. The red atoms are In, and the blue atoms are Sb. (j) also displays how a leading partial dislocation and trailing partial dislocation merge into a perfect dislocation. Notice that neither the trailing partial dislocation in (h), (i) or the perfect dislocation in (k), (l), (m) are parallel to the paper, which is clearly shown in (j) and (n).



Supplementary Figure 3| Models of shear response calculations. Four models used to examine shear response along various slip systems. (a) [100]×[010]×[001] model. (b) [110]×[1$\bar{1}$0]×[00$\bar{1}$] model. (c) [11$\bar{2}$]×[111]×[1$\bar{1}$0] model. (d) [11$\bar{1}$]×[123]×[5$\bar{4}$1] model. The red atoms are In, and the blue atoms are Sb.